Sharp Transition for Single Polarons in the One-Dimensional Su-Schrieffer-Heeger Model

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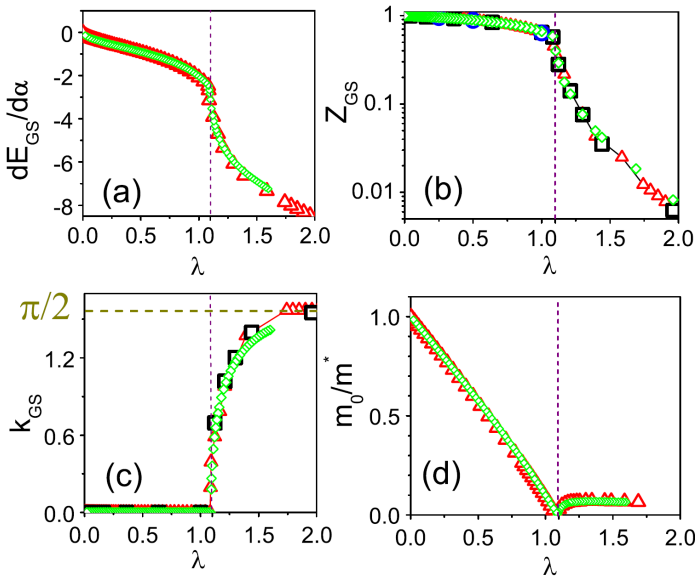
Polarons have been of broad interest in physics ever since they were introduced in 1933 and, apart the their central role in solid state physics, they exemplify in quantum field theory the passage from weak to strong coupling in a non trivial model of a single particle coupled to a bosonic field. In the paper we have studied a single polaron in the Su-Schrieffer-Heeger (SSH) model by using four different techniques (three numerical and one analytical). We show that the model exhibits sharp transition, at a critical coupling strength λc, between states with zero and nonzero momentum of the ground state. This results is unexpected since polarons show a smooth crossover from weak to strong coupling, as a function of the electron-phonon coupling strength λ, in all models where this coupling depends only on phonon momentum q.



Our result prove that in models where the coupling depends also on the electron momentum k, as in the SSH model, the physics of the intermediate regime is very different. This result is representative of all polarons with coupling depending on k and q, and can have important experimental consequences (e.g., in angle-resolved photoemission spectroscopy and conductivity experiments). Within this collaboration, in particular CNR-SPIN research unit developed the Limited Phonon Basis Exact Diagonalization that has been successfully applied also to other models in different contexts.

Derivative of the GS energy with respect to α, (b) Z factor of the GS, (c) wave vector of the GS, and (d) the ratio m_0/m^* of the bare and effective polaronic masses at K_{GS} for ω_{ph}=0.5. Red triangles, green rhombi, black squares, and blue circles correspond to LPBED, MA, DMC, and BDMC methods, respectively. The vertical dashed line indicates the critical coupling λ_c.